ADVANCES IN SURFACE-ENHANCED RAMAN SPECTROSCOPY FOR APPLICATIONS IN REAL-TIME SUBSURFACE MONITORING*

Eric A. Wachter
T. L. Ferrell
R. B. Gammage
T. Vo-Dinh
J. W. Haas, III
D. R. James
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831-6113

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TITLE: ADVANCES IN SURFACE-ENHANCED RAMAN SPECTROSCOPY FOR APPLICATIONS IN REAL-TIME SUBSURFACE MONITORING

SITE OR LOCATION OF PROJECT: ORNL

PROJECT OBJECTIVE:

Because of its excellent selectivity and high sensitivity, surface enhanced Raman scattering (SERS) has attracted considerable attention as a potentially powerful analytical tool for detection and screening of trace-level contaminants in groundwater. The narrow Raman bands hold promise for simplifying the identification of individual components in complex mixtures.

APPROACH:

An inexpensive computer-controlled portable spectrometer system coupled to a fiberoptic probe is being developed for rapid on-site and *in situ* determination of organic groundwater contamination. Novel substrates are being investigated as a means for increasing the sensitivity of the SERS technique. Critical issues pertaining to durability, repeatability, sensitivity, selectivity and universality are being examined, while means for improvement in these areas are being tested.

RESULTS:

Progress at ORNL has demonstrated feasibility of utilizing SERS under harsh conditions, as well as tailoring of substrates for maximum effeciency with particular excitation wavelengths. Several new substrate materials have been developed. Ongoing efforts have refined the state-of-the-art in Raman optrode design, and have shown feasibility of producing a simple, inexpensive instrument for field applications.

BENEFITS:

As the technique approaches maturity, SERS will provide powerful screening capabilities for numerous organic and inorganic materials. SERS promises rapid, reproducible, quantitative detection of trace-level contaminats in aqueous solution.

PRINCIPLE INVESTIGATORS:

E.A. Wachter	615/574-6248 (FTS-624-6248)
T.L. Ferrell	615/574-6214 (FTS-624-6214)
R.B. Gammage	615/574-6256 (FTS-624-6256)
T. Vo-Dinh	615/574-6249 (FTS-624-6249)
J.W. Haas, III	615/574-5042 (FTS-624-5042)
D.R. James	615/574-6213 (FTS-624-6213)

Health and Safety Research Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831

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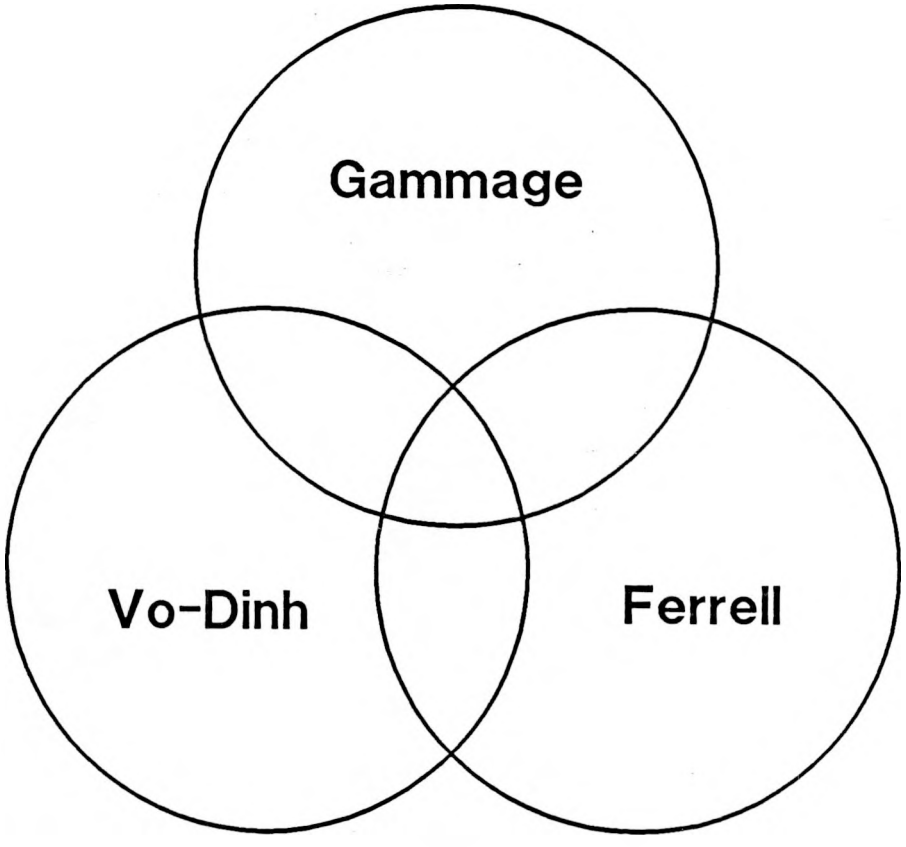
Eric Wachter, Ph.D.

Health and Safety Research Division
Oak Ridge National Laboratory

ORNL SERS Initiative



ORNL SERS RESEARCH

- SUBSTRATE DEVELOPMENT

- PROBE DESIGN

- PORTABLE INSTRUMENTS

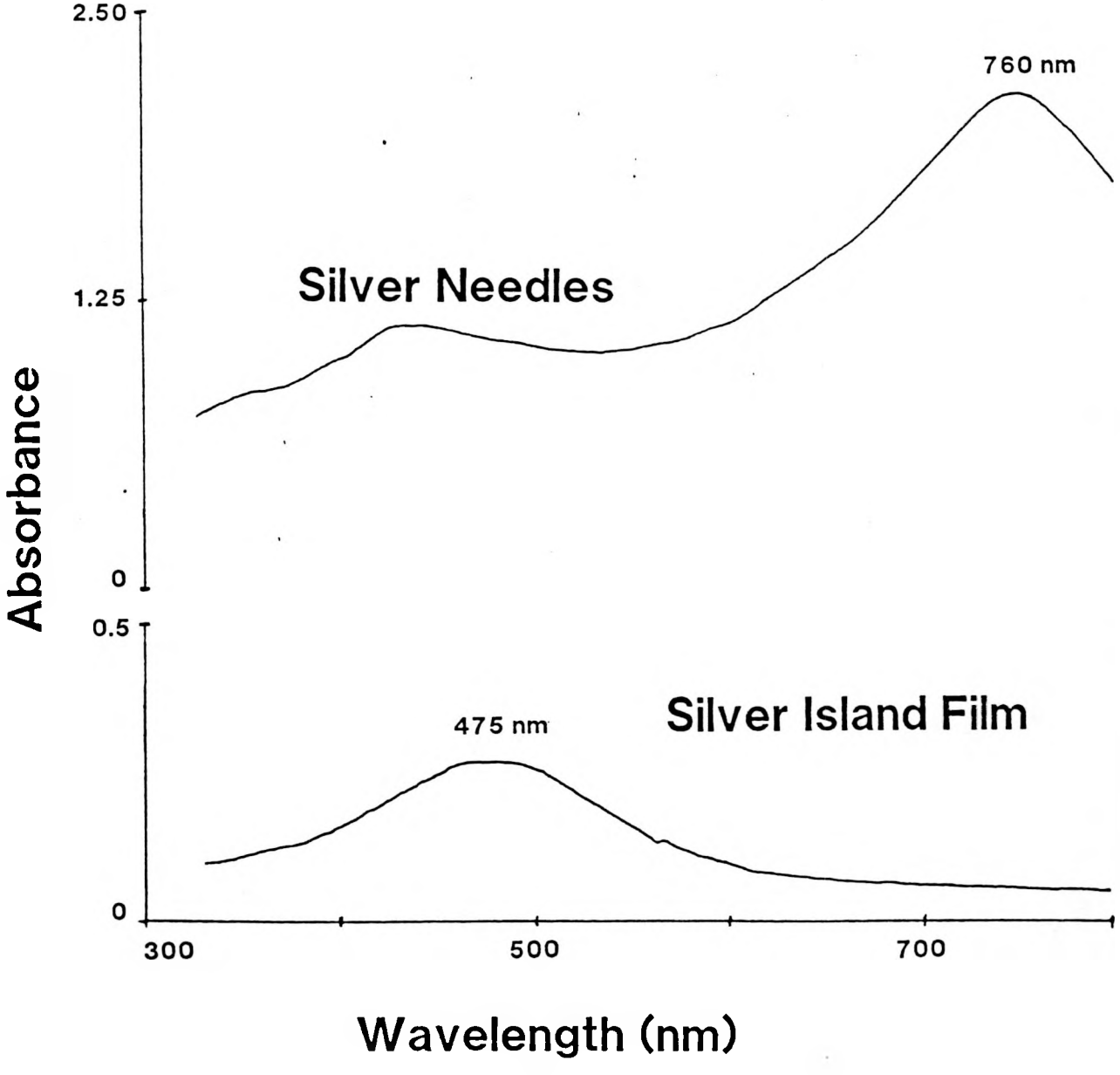
ORNL SERS RESEARCH

- SUBSTRATE DEVELOPMENT

- MICROBODIES

- MICROLITHOGRAPHIC STRUCTURES

- COLUMNAR METAL BODIES (NEEDLES)


2.50
1.25
0
0.5
0
760 nm
Silver Needles
475 nm
Silver Island Film
Absorbance
300
500
700
Wavelength (nm)

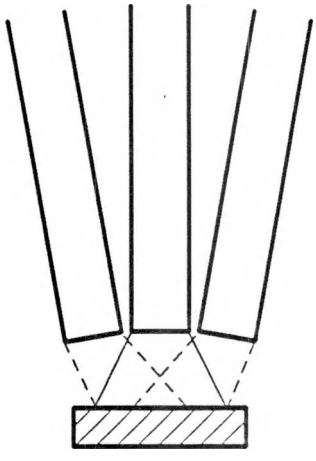
CRITICAL PARAMETERS IN OPTRODE DESIGN

- BACKSCATTERING GEOMETRY
- SIMPLE OPTICS
- SMALL
- MODULAR
- HIGH EXCITATION EFFICIENCY
- HIGH COLLECTION EFFICIENCY
- ACHROMATIC
- LONG FOCAL LENGTH
- EASILY FILTERED

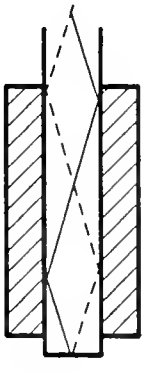
PROBE GEOMETRIES

INTERNAL BACKSCATTERING

EXTERNAL BACKSCATTERING

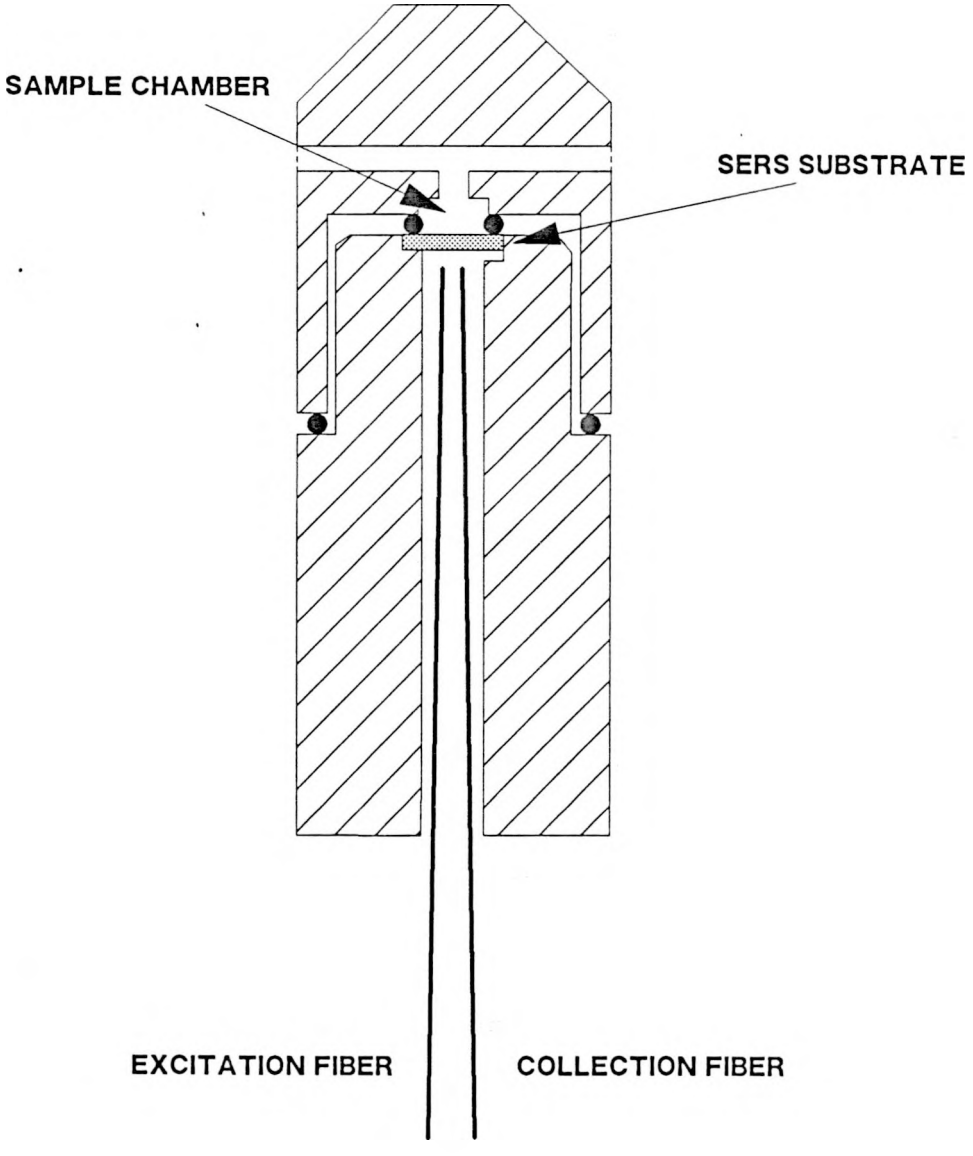


INTERNAL EVANESCENCE

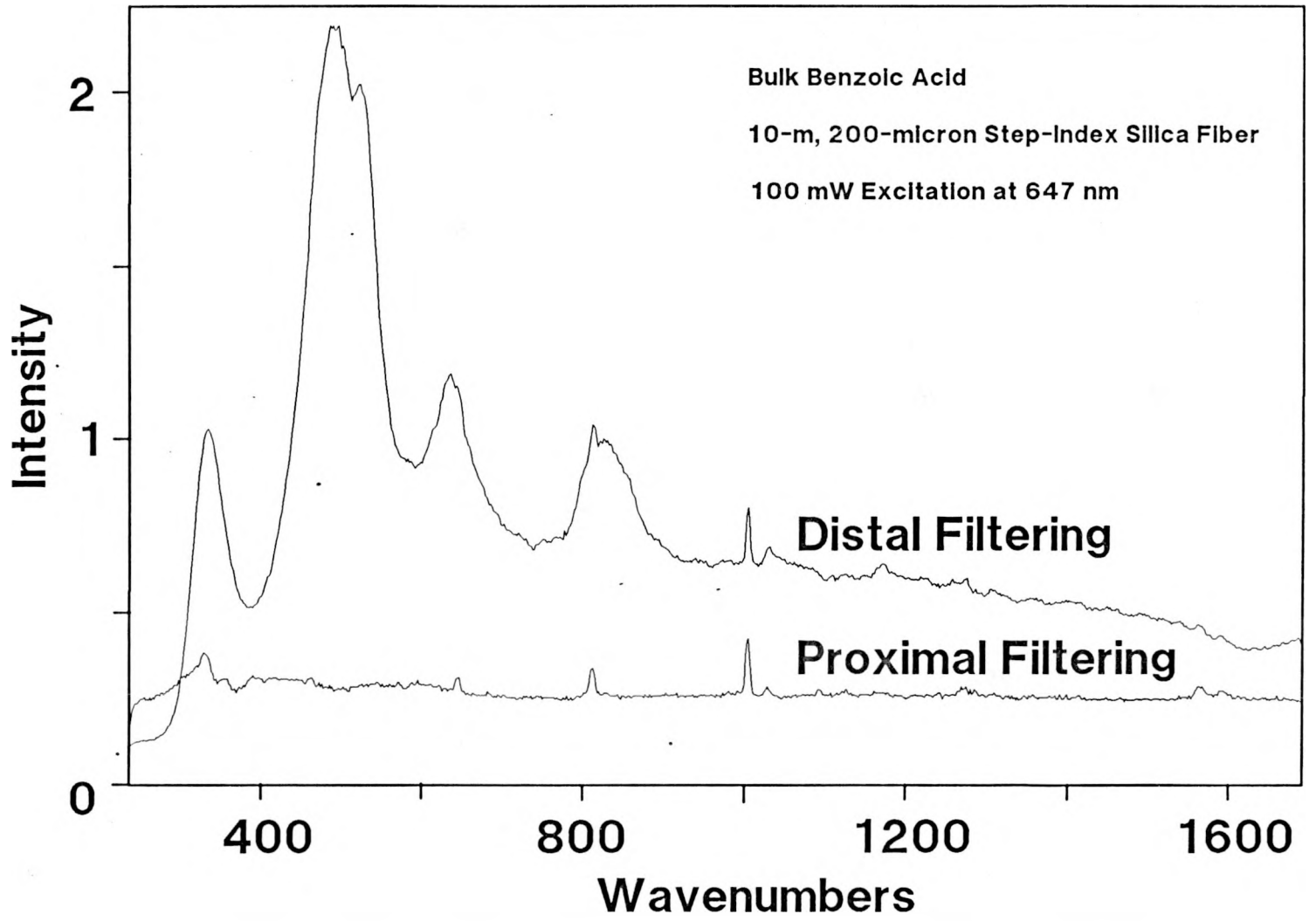


PASS-THRU

INITIAL SERS FIBEROPTIC PROBE

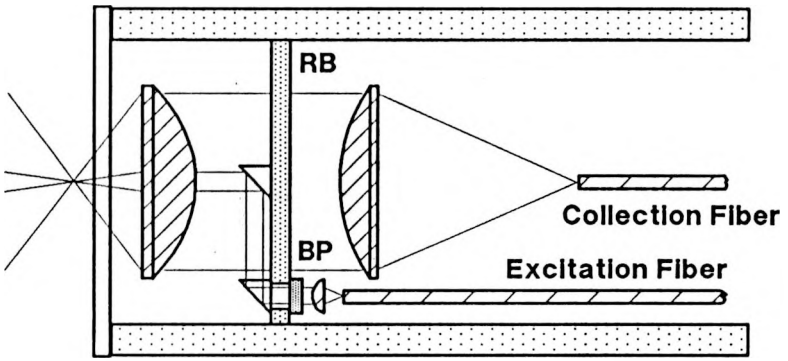


Effect of Filter Position for Fiberoptic Collection of Raman Scattering

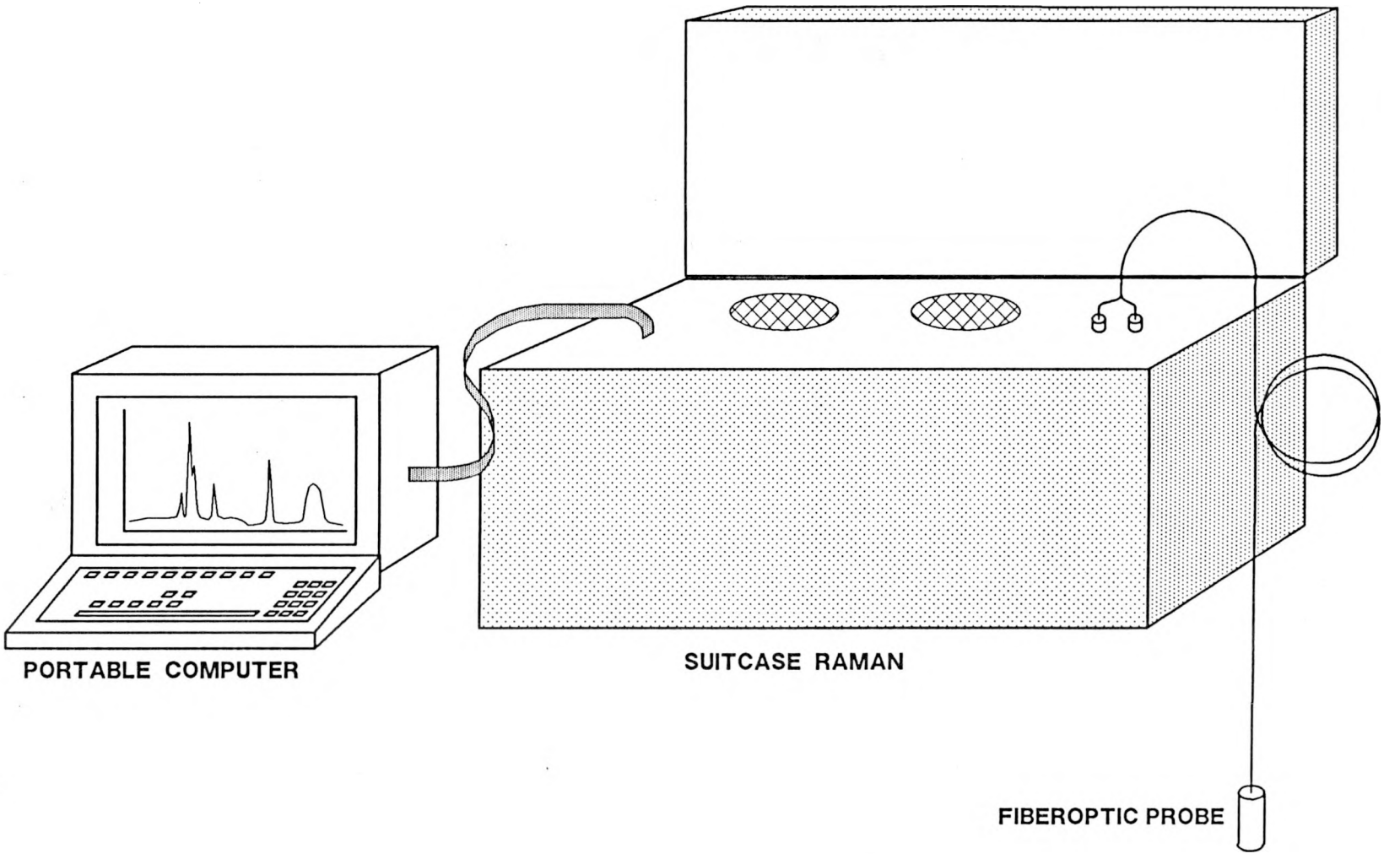


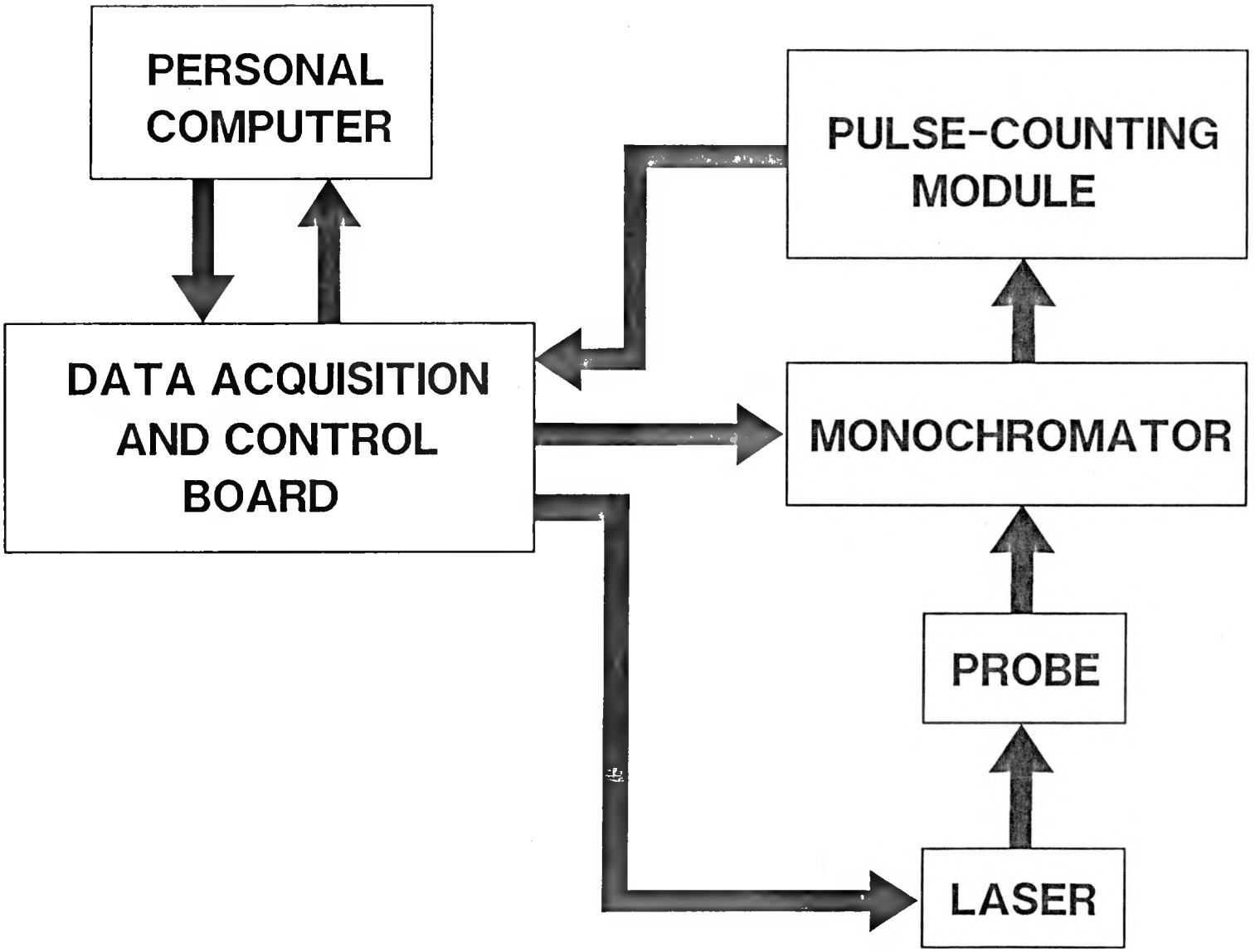
	BARE FIBER	GRIN LENS	STD LENS
COMPLEXITY	simple	simple	complex
SIZE	very small	small	small to large
COST	low	moderate	high
EFFICIENCY	very low	low to high	very high
VERSATILITY	interferences very short focal length	limited wavelengths chromatic errors limited focal lengths limited N.A.	broadband applicability low chromatic effects many focal lengths many N.A.'s
P/PR	poor	moderate	high

BACK-SCATTERING RAMAN PROBE



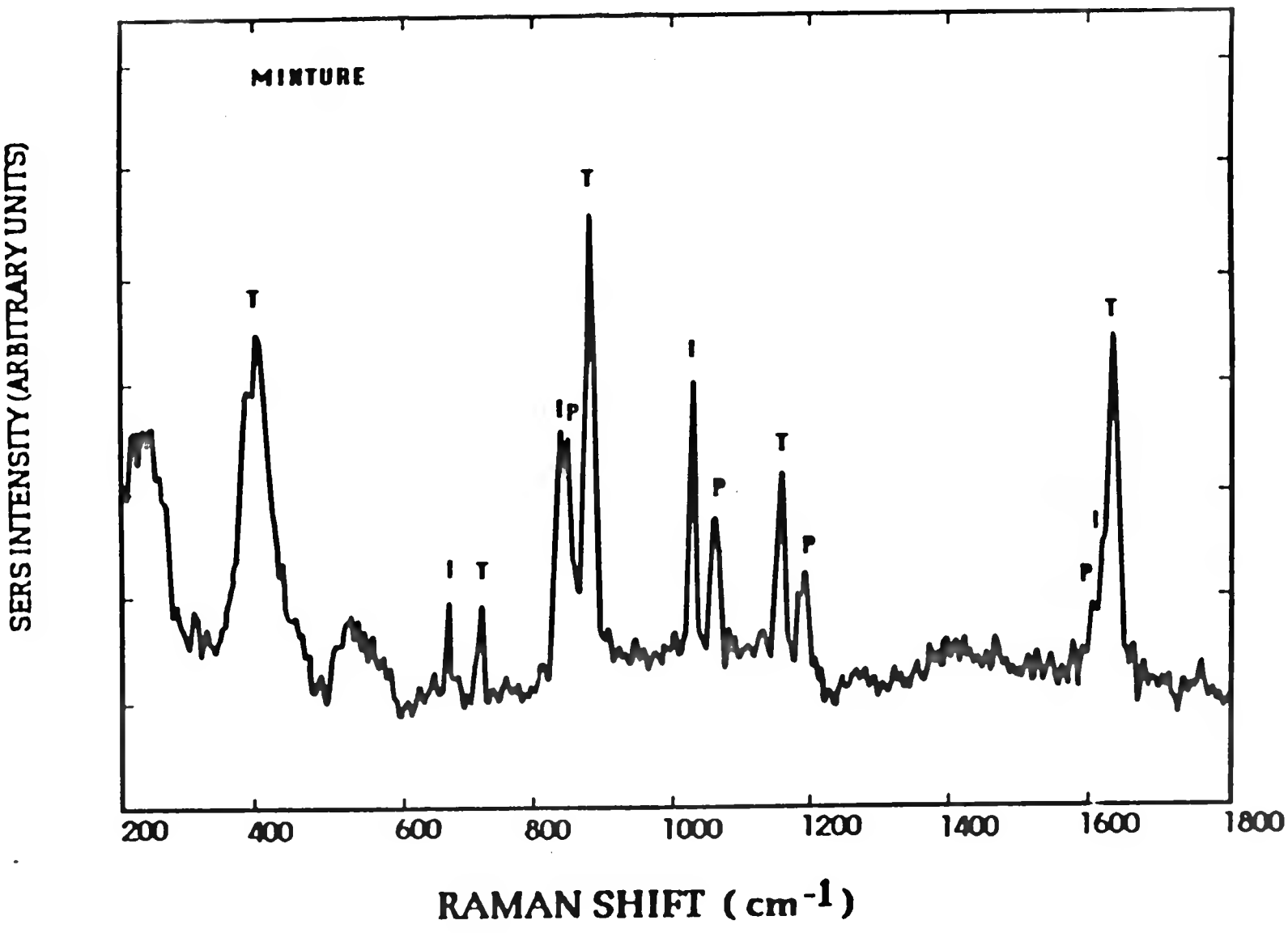
FIELD-PORTABLE RAMAN SYSTEM




PERSONAL COMPUTER
PULSE-COUNTING MODULE
DATA ACQUISITION AND CONTROL BOARD
MONOCHROMATOR
PROBE
LASER

CRITICAL AREAS

- ADSORPTION CONTROL
- CHEMICAL ENHANCEMENT
- INSTRUMENT/PROBE PORTABILITY
- SPEED OF ANALYSIS


MIXTURE
SERS INTENSITY (ARBITRARY UNITS)
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200
400
600
800
1000
1200
1400
1600
1800
RAMAN SHIFT (cm-1)